Vertical balance equations

Benjamin Ménétrier

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Contents

1 Block formulation

Let $\mathbf{x} \in \mathbb{R}^n$ be the "balanced variable" and $\mathbf{v} \in \mathbb{R}^n$ be the "unbalanced variable". They are linked through a "balance operator" $\mathbf{K} \in \mathbb{R}^{n \times n}$:

$$\mathbf{x} = \mathbf{K}\mathbf{v} \tag{1}$$

Let split $\mathbf{x}$ and $\mathbf{v}$ into m blocks, and $\mathbf{K}$ into m^2 square blocks:

$$\begin{pmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_m \end{pmatrix} = \begin{pmatrix} \mathbf{K}_{1,1} & \dots & \mathbf{K}_{1,m} \\ \vdots & \ddots & \vdots \\ \mathbf{K}_{m,1} & \dots & \mathbf{K}_{m,m} \end{pmatrix} \begin{pmatrix} \mathbf{v}_1 \\ \vdots \\ \mathbf{v}_m \end{pmatrix} \tag{2}$$

or

$$\mathbf{x}_i = \sum_{j=1}^{m} \mathbf{K}_{i,j} \mathbf{v}_j \tag{3}$$

where the size of each sub-vector $\mathbf{x}_i$ and $\mathbf{v}_i$ is n_i, with $\sum_{i=1}^{m} n_i = n$, and $\mathbf{K}_{i,j} \in \mathbb{R}^{n_i \times n_j}$.

2 Triangular assumption

We assume that the balance operator $\mathbf{K}$ is block-lower-triangular, with identity diagonal blocks:

$$\mathbf{K} = \begin{pmatrix} \mathbf{I}_{n_1} & 0 & \dots & \dots & 0 \\ \mathbf{K}_{2,1} & \mathbf{I}_{n_2} & \ddots & & \vdots \\ \mathbf{K}_{3,1} & \mathbf{K}_{3,2} & \mathbf{I}_{n_3} & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ \mathbf{K}_{m,1} & \mathbf{K}_{m,2} & \dots & \mathbf{K}_{m,m-1} & \mathbf{I}_{n_m} \end{pmatrix} \tag{4}$$

Thus, we can simplify equation (3) into:

$$\mathbf{x}_i = \sum_{j=1}^{i-1} \mathbf{K}_{i,j} \mathbf{v}_j + \mathbf{v}_i \tag{5}$$

3 Adjoint

The adjoint of the balance operator is given by:

$$\mathbf{K}^{\mathrm{T}} = \begin{pmatrix} \mathbf{I}_{n_1} & \mathbf{K}^{\mathrm{T}}_{2,1} & \mathbf{K}^{\mathrm{T}}_{3,1} & \dots & \mathbf{K}^{\mathrm{T}}_{m,1} \\ 0 & \mathbf{I}_{n_2} & \mathbf{K}^{\mathrm{T}}_{3,2} & \dots & \mathbf{K}^{\mathrm{T}}_{m,2} \\ \vdots & \ddots & \mathbf{I}_{n} & \ddots & \vdots \\ \vdots & & \ddots & \ddots & \mathbf{K}^{\mathrm{T}}_{m,m-1} \\ 0 & \dots & \dots & 0 & \mathbf{I}_{n_m} \end{pmatrix} \tag{6}$$

so $\mathbf{v} = \mathbf{K}^{\mathrm{T}}\mathbf{x}$ can be expressed as:

$$\mathbf{v}_i = \mathbf{x}_i + \sum_{j=i+1}^{m} \mathbf{K}_{j,i}^{\mathrm{T}} \mathbf{x}_j \tag{7}$$

4 Partial recursive inverse

Equation (5) can be transformed to compute $\mathbf{v}$ knowing $\mathbf{x}$ recursively:

$$\mathbf{v}_i = \mathbf{x}_i - \sum_{j=1}^{i-1} \mathbf{K}_{i,j} \mathbf{v}_j \tag{8}$$

It should be noted that the inverse of $\mathbf{K}_{i,j}$ is not required. This inverse formula is refered to as "partial" since the unbalanced variable $\mathbf{v}$ still appears on the right-hand side.

For the adjoint in equation (7), the same transformation leads to:

$$\mathbf{x}_i = \mathbf{v}_i - \sum_{j=i+1}^{m} \mathbf{K}_{j,i}^{\mathrm{T}} \mathbf{x}_j \tag{9}$$

and must be applied recursively in reverse order (i from m to 1).

5 Full recursive inverse

We assume that for $1 \leq j \leq i$, there are matrices $\mathbf{A}_{i,j} \in \mathbb{R}^{n_i \times n_j}$ such that $\mathbf{v}_i$ can be expressed only as a function of $\mathbf{x}$:

$$\mathbf{v}_i = \sum_{j=1}^{i} \mathbf{A}_{i,j} \mathbf{x}_j \tag{10}$$

Plugging this expression into the partial recursive inverse formula (8), we get:

$$\begin{aligned}
\mathbf{v}_i &= \mathbf{x}_i - \sum_{j=1}^{i-1} \mathbf{K}_{i,j} \mathbf{v}_j \\
&= \mathbf{x}_i - \sum_{j=1}^{i-1} \sum_{k=1}^{j} \mathbf{K}_{i,j} \mathbf{A}_{j,k} \mathbf{x}_k \\
&= \mathbf{x}_i - \sum_{k=1}^{i-1} \sum_{j=k}^{i-1} \mathbf{K}_{i,j} \mathbf{A}_{j,k} \mathbf{x}_k \\
&= \mathbf{x}_i - \sum_{j=1}^{i-1} \sum_{k=j}^{i-1} \mathbf{K}_{i,k} \mathbf{A}_{k,j} \mathbf{x}_j \\
&= \sum_{j=1}^{i-1} \left(- \sum_{k=j}^{i-1} \mathbf{K}_{i,k} \mathbf{A}_{k,j} \right) \mathbf{x}_j + \mathbf{x}_i
\end{aligned} \tag{11}$$

which is consistent with (10) if:

$$\mathbf{A}_{i,j} = -\sum_{k=j}^{i-1} \mathbf{K}_{i,k}\mathbf{A}_{k,j} \text{ (for } j < i\text{)} \tag{12a}$$

$$\mathbf{A}_{i,i} = \mathbf{I}_{n_i} \tag{12b}$$

For convenience, we also define the matrices $\mathbf{A}_{i,j}$ for $j > i$ to make the full matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$:

$$\mathbf{A}_{i,j} = \mathbf{A}_{j,i}^{\mathrm{T}} \tag{13}$$

6 Sequential estimation

Since $\mathbf{v}$ is an "unbalanced variable", the component $\mathbf{v}_i$ should be uncorrelated with all the other components:

$$\text{if } j \neq i,\ \operatorname{Cov}\left(\mathbf{v}_i, \mathbf{v}_j\right) = 0 \tag{14}$$

Using the partial recursive inverse (8) for $j < i$, we get:

$$\begin{aligned}
&\operatorname{Cov}\left(\mathbf{v}_i, \mathbf{v}_j\right) = 0 \\
\Leftrightarrow\ &\operatorname{Cov}\left(\mathbf{x}_i - \sum_{k=1}^{i-1} \mathbf{K}_{i,k}\mathbf{v}_k, \mathbf{v}_j\right) = 0 \\
\Leftrightarrow\ &\operatorname{Cov}\left(\mathbf{x}_i, \mathbf{v}_j\right) - \sum_{k=1}^{i-1} \mathbf{K}_{i,k} \operatorname{Cov}\left(\mathbf{v}_k, \mathbf{v}_j\right) = 0
\end{aligned} \tag{15}$$

Using the statistical property (14) of $\mathbf{v}$, the term for which $k = j$ is the only one remaining:

$$\begin{aligned}
\operatorname{Cov}\left(\mathbf{x}_i, \mathbf{v}_j\right) - \mathbf{K}_{i,j} \operatorname{Cov}\left(\mathbf{v}_j, \mathbf{v}_j\right) &= 0 \\
\mathbf{K}_{i,j} = \operatorname{Cov}\left(\mathbf{x}_i, \mathbf{v}_j\right) \operatorname{Cov}\left(\mathbf{v}_j, \mathbf{v}_j\right)^{-1} &
\end{aligned} \tag{16}$$

Using the full recursive inverse (10), we get for $j < i$:

$$\begin{aligned}
\operatorname{Cov}\left(\mathbf{x}_i, \mathbf{v}_j\right) &= \operatorname{Cov}\left(\mathbf{x}_i, \sum_{k=1}^{j} \mathbf{A}_{j,k}\mathbf{x}_k\right) \\
&= \sum_{k=1}^{j} \operatorname{Cov}\left(\mathbf{x}_i, \mathbf{x}_k\right) \mathbf{A}_{j,k}^{\mathrm{T}}
\end{aligned} \tag{17a}$$

$$\begin{aligned}
\operatorname{Cov}\left(\mathbf{v}_j, \mathbf{v}_j\right) &= \operatorname{Cov}\left(\sum_{k=1}^{j} \mathbf{A}_{j,k}\mathbf{x}_k, \sum_{l=1}^{j} \mathbf{A}_{j,l}\mathbf{x}_l\right) \\
&= \sum_{k=1}^{j} \mathbf{A}_{j,k} \sum_{l=1}^{j} \operatorname{Cov}\left(\mathbf{x}_k, \mathbf{x}_l\right) \mathbf{A}_{j,l}^{\mathrm{T}}
\end{aligned} \tag{17b}$$

which allows a computation of the balance operator $\mathbf{K}_{i,j}$ using expression (16).

7 Aggregated formulation

For practical reasons explained later in section 8, we define aggregated quantities:

- the aggregated size $\bar{n}_i = \sum_{j=1}^{i-1} n_j$
- the aggregated vectors $\bar{\mathbf{x}}_i$ and $\bar{\mathbf{v}}_i \in \mathbb{R}^{\bar{n}_i}$:

$$\bar{\mathbf{x}}_i = \begin{pmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_{i-1} \end{pmatrix} \text{ and } \bar{\mathbf{v}}_i = \begin{pmatrix} \mathbf{v}_1 \\ \vdots \\ \mathbf{v}_{i-1} \end{pmatrix} \tag{18}$$

- the aggregated operator $\overline{\mathbf{K}}_i \in \mathbb{R}^{n_i \times \bar{n}_i}$:

$$\overline{\mathbf{K}}_i = \begin{pmatrix} \mathbf{K}_{i,1} & \dots & \mathbf{K}_{i,i-1} \end{pmatrix} \tag{19}$$

- the aggregated matrix $\overline{\mathbf{A}}_i \in \mathbb{R}^{n_i \times \bar{n}_i}$:

$$\overline{\mathbf{A}}_i = \begin{pmatrix} \mathbf{A}_{i,1} & \dots & \mathbf{A}_{i,i-1} \end{pmatrix} \tag{20}$$

Thus, equation (5) can be rewritten as:

$$\mathbf{x}_i = \overline{\mathbf{K}}_i \bar{\mathbf{v}}_i + \mathbf{v}_i \tag{21}$$

The partial inverse formulation (8) can be rewritten as:

$$\mathbf{v}_i = \mathbf{x}_i - \overline{\mathbf{K}}_i \bar{\mathbf{v}}_i \tag{22}$$

and the full inverse formulation (10) can be rewritten as:

$$\mathbf{v}_i = \overline{\mathbf{A}}_i \bar{\mathbf{x}}_i + \mathbf{x}_i \tag{23}$$

with $\mathbf{A}_{i,j}$ computed as:

$$\mathbf{A}_{i,j} = -\overline{\mathbf{K}}_i \overline{\mathbf{A}}_j^{\mathrm{T}} \tag{24}$$

Finally, we define the matrix $\overline{\overline{\mathbf{A}}}_i \in \mathbb{R}^{\bar{n}_i \times \bar{n}_i}$:

$$\overline{\overline{\mathbf{A}}}_i = \begin{pmatrix} \mathbf{I} & 0 & \dots & 0 \\ \mathbf{A}_{2,1} & \mathbf{I} & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ \mathbf{A}_{\mathbf{i-1,1}} & \dots & \mathbf{A}_{\mathbf{i-1,i-2}} & \mathbf{I} \end{pmatrix} \tag{25}$$

to get the aggregated form:

$$\bar{\mathbf{v}}_i = \bar{\bar{\mathbf{A}}}_i \bar{\mathbf{x}}_i \tag{26}$$

The assumption (14) can be rewritten as:

$$\mathrm{Cov}\left(\mathbf{v}_i, \bar{\mathbf{v}}_i\right) = 0 \tag{27}$$

leading to the equivalent of equation (16):

$$\overline{\mathbf{K}}_i = \mathrm{Cov}\left(\mathbf{x}_i, \bar{\mathbf{v}}_i\right) \mathrm{Cov}\left(\bar{\mathbf{v}}_i, \bar{\mathbf{v}}_i\right)^{-1} \tag{28}$$

Expanding eqation (27) with the partial recursive inverse (22) we get:

$$\begin{aligned}
& \mathrm{Cov}\left(\mathbf{v}_i, \bar{\mathbf{v}}_i\right) = 0 \\
\Leftrightarrow\ & \mathrm{Cov}\left(\mathbf{x}_i - \overline{\mathbf{K}}_i \bar{\mathbf{v}}_i, \bar{\mathbf{v}}_i\right) = 0 \\
\Leftrightarrow\ & \mathrm{Cov}\left(\mathbf{x}_i, \bar{\mathbf{v}}_i\right) - \overline{\mathbf{K}}_i \mathrm{Cov}\left(\bar{\mathbf{v}}_i, \bar{\mathbf{v}}_i\right) = 0 \\
\Leftrightarrow\ & \overline{\mathbf{K}}_i = \mathrm{Cov}\left(\mathbf{x}_i, \bar{\mathbf{v}}_i\right) \mathrm{Cov}\left(\bar{\mathbf{v}}_i, \bar{\mathbf{v}}_i\right)^{-1}
\end{aligned} \tag{29}$$

Using the aggregated full recursive inverse (23) and the aggregated form (26), we get:

$$\begin{aligned}
\mathrm{Cov}\left(\mathbf{x}_i, \bar{\mathbf{v}}_i\right) &= \mathrm{Cov}\left(\mathbf{x}_i, \bar{\bar{\mathbf{A}}}_i \bar{\mathbf{x}}_i\right) \\
&= \mathrm{Cov}\left(\mathbf{x}_i, \bar{\mathbf{x}}_i\right) \bar{\bar{\mathbf{A}}}_i^{\mathrm{T}}
\end{aligned} \tag{30a}$$

$$\begin{aligned}
\mathrm{Cov}\left(\bar{\mathbf{v}}_i, \bar{\mathbf{v}}_i\right) &= \mathrm{Cov}\left(\bar{\bar{\mathbf{A}}}_i \bar{\mathbf{x}}_i, \bar{\bar{\mathbf{A}}}_i \bar{\mathbf{x}}_i\right) \\
&= \bar{\bar{\mathbf{A}}}_i \mathrm{Cov}\left(\bar{\mathbf{x}}_i, \bar{\mathbf{x}}_i\right) \bar{\bar{\mathbf{A}}}_i^{\mathrm{T}}
\end{aligned} \tag{30b}$$

which allows a computation of the balance operator $\overline{\mathbf{K}}_i$ using expression (29).

8 Practical computations

In practice, covariances are sampled from an ensemble. Let $\left\{\widetilde{\mathbf{x}}^1, \dots, \widetilde{\mathbf{x}}^N\right\}$ be a set of N vectors that samples the distribution of $\mathbf{x}$ and $\left\{\delta\widetilde{\mathbf{x}}^1, \dots, \delta\widetilde{\mathbf{x}}^N\right\}$ their centered counterparts:

$$\delta\widetilde{\mathbf{x}}^p = \widetilde{\mathbf{x}}^p - \langle\widetilde{\mathbf{x}}\rangle \tag{31}$$

where $\langle\cdot\rangle$ denotes the ensemble mean:

$$\langle\widetilde{\mathbf{x}}\rangle = \frac{1}{N}\sum_{p=1}^{N} \widetilde{\mathbf{x}}^p \tag{32}$$

The covariance $\mathrm{Cov}\left(\mathbf{x}_i, \mathbf{x}_j\right)$ can be estimated from these perturbations by:

$$\widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{x}_j\right) = \frac{1}{N-1}\sum_{p=1}^{N} \delta\widetilde{\mathbf{x}}_i^p \left(\delta\widetilde{\mathbf{x}}_j^p\right)^{\mathrm{T}} \tag{33}$$

Because of the limited ensemble size N, it can be relevant to filter the covariance matrix with a linear operator $\mathcal{F}$:

$$\widehat{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{x}_j\right) = \mathcal{F}\left[\widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{x}_j\right)\right] \tag{34}$$

Since regressions are estimated with approximate covariances, the non-aggregated and the aggregated formulations give different results in practice. Indeed, the aggregated formulation will actually compute the cross-covariances between unbalanced variables (non-diagonal blocks) in $\widehat{\mathrm{Cov}}\left(\bar{\mathbf{v}}_i, \bar{\mathbf{v}}_i\right)$, whereas the non-aggregated formulation assumes that $\widehat{\mathrm{Cov}}\left(\bar{\mathbf{v}}_i, \bar{\mathbf{v}}_i\right)$ is block-diagonal. Hereafter, we describe calculations for the aggregated formulation. The non-aggregated formulation is simply obtained by forcing non-diagonal block to zero in $\widehat{\mathrm{Cov}}\left(\bar{\mathbf{v}}_i, \bar{\mathbf{v}}_i\right)$.

The computation of the balance operator components using the partial recursive inverse equation (22) is detailed in algorithm 1. Its counterpart using the full recursive inverse equation (23) is detailed in algorithm 2. It should be noted that algorithm 1 requires storing the ensemble twice, while algorithm 2 requires storing more matrices.

9 Time-averaging

Let's assume that we have several occurences of an ensemble for different dates/times. A sliding average, possibly with different weights, sounds like a reasonable idea to increase the sampling size and reduce the sampling noise. However, this should be done carefully:

- Since regressions $\mathbf{K}_{i,j}$ are ratios of covariances, it is not relevant to average them overtime. Moreover, as shown in section 10, regressions can be very sensitive to sampling noise and their estimation very unstable.

- Covariances $\widehat{\mathrm{Cov}}\left(\mathbf{x}_i, \bar{\mathbf{v}}_i\right)$ and $\widehat{\mathrm{Cov}}\left(\bar{\mathbf{v}}_i, \bar{\mathbf{v}}_i\right)$ involve unbalanced covariances, that are comp$\mathbf{K}_{i,j}$ dependent on the sequential computation of regressions, so they should be not be averaged neither.

- Only the covariances $\widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{x}_j\right)$ are actual covariances of balanced variables, that can be averaged safely. Thus, only the full recursive inverse formula should be used to compute time-averaged regressions, as shown in algorithm 3.

10 Regression estimation error

To characterize theoretically the error arising when estimating a regression operator, we define the simplest possible framework. The background error covariance matrix $\mathbf{B} \in \mathbb{R}^{2\times 2}$ is defined as:

$$\mathbf{B} = \mathbf{K}\mathbf{C}_u\mathbf{K}^{\mathrm{T}} \tag{35}$$

where $\mathbf{K} \in \mathbb{R}^{2\times 2}$ is defined by a scalar regression r:

$$\mathbf{K} = \begin{pmatrix} 1 & 0 \\ r & 1 \end{pmatrix} \tag{36}$$

and $\mathbf{C}_u \in \mathbb{R}^{2\times 2}$ is the diagonal matrix of variances:

$$\mathbf{C}_u = \begin{pmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{pmatrix} \tag{37}$$

Thus:

$$\mathbf{B} = \begin{pmatrix} \sigma_1^2 & r\sigma_1^2 \\ r\sigma_1^2 & r^2\sigma_1^2 + \sigma_2^2 \end{pmatrix} \tag{38}$$

and the correlation matrix is given by:

$$\mathbf{C} = \begin{pmatrix} 1 & c \\ c & 1 \end{pmatrix} \tag{39}$$

with:

$$\begin{aligned} c &= \frac{r\sigma_1}{\sqrt{r^2\sigma_1^2 + \sigma_2^2}} \\ &= \left(1 + \left(\frac{\sigma_2}{r\sigma_1}\right)^2\right)^{-1/2} \end{aligned} \tag{40}$$

A possible square-root of $\mathbf{B}$ is $\mathbf{U} \in \mathbb{R}^{2\times 2}$:

$$\mathbf{U} = \begin{pmatrix} \sigma_1 & 0 \\ r\sigma_1 & \sigma_2 \end{pmatrix} \tag{41}$$

We assume that an ensemble of N perturbations $\boldsymbol{\zeta}$ is generated by randomization:

$$\begin{aligned} \boldsymbol{\zeta} &= \mathbf{U}\boldsymbol{\eta} \\ &= \begin{pmatrix} \sigma_1\eta_1 \\ r\sigma_1\eta_1 + \sigma_2\eta_2 \end{pmatrix} \end{aligned} \tag{42}$$

where $\boldsymbol{\eta} \in \mathbb{R}^2$ is a Gaussian deviate of zero mean and unit variance: $\boldsymbol{\eta} \sim \mathcal{N}\left(0, \mathbf{I}_2\right)$.

The regression coefficient r is estimated as:

$$
\begin{aligned}
\widetilde{r} &= \frac{\widetilde{\mathrm{Cov}}\left(\zeta_2, \zeta_1\right)}{\widetilde{\mathrm{Var}}\left(\zeta_1\right)} \\
&= \frac{r\sigma_1^2\widetilde{\mathrm{Var}}\left(\eta_1\right) + \sigma_1\sigma_2\widetilde{\mathrm{Cov}}\left(\eta_2, \eta_1\right)}{\sigma_1^2\widetilde{\mathrm{Var}}\left(\eta_1\right)} \\
&= r + \frac{\sigma_2\widetilde{\mathrm{Cov}}\left(\eta_2, \eta_1\right)}{\sigma_1\widetilde{\mathrm{Var}}\left(\eta_1\right)}
\end{aligned}
\tag{43}
$$

Thus, the estimation error on r is:

$$
\widetilde{r} - r = \frac{\sigma_2\widetilde{\mathrm{Cov}}\left(\eta_2, \eta_1\right)}{\sigma_1\widetilde{\mathrm{Var}}\left(\eta_1\right)}
\tag{44}
$$

Due to the limited sample size, the estimations are noisy:

$$
\widetilde{\mathrm{Cov}}\left(\eta_2, \eta_1\right) = \mathrm{Cov}\left(\eta_2, \eta_1\right) + \varepsilon_{21}
\tag{45a}
$$

$$
\widetilde{\mathrm{Var}}\left(\eta_1\right) = \mathrm{Var}\left(\eta_1\right) + \varepsilon_1
\tag{45b}
$$

where the definition of $\boldsymbol{\eta}$ yields:

$$
\mathrm{Cov}\left(\eta_2, \eta_1\right) = 0
\tag{46a}
$$

$$
\mathrm{Var}\left(\eta_1\right) = 1
\tag{46b}
$$

and the covariance estimation theory gives:

$$
\mathbb{E}\left[\varepsilon_{21}\right] = 0
\tag{47a}
$$

$$
\mathrm{Var}\left(\varepsilon_{21}^2\right) = \frac{1}{N-1}
\tag{47b}
$$

and

$$
\mathbb{E}\left[\varepsilon_1\right] = 0
\tag{48a}
$$

$$
\mathrm{Var}\left(\varepsilon_1^2\right) = \frac{2}{N-1}
\tag{48b}
$$

If N is large enough, $\varepsilon_1 \ll 1$ so:

$$
\frac{1}{\widetilde{\mathrm{Var}}\left(\eta_1\right)} = \frac{1}{1+\varepsilon_1} \simeq 1 - \varepsilon_1
\tag{49}
$$

and $\varepsilon_{21} \ll 1$ also, leading to a first order approximation:

$$\widetilde{r} - r \simeq \frac{\sigma_2}{\sigma_1}\varepsilon_{21}\left(1 - \varepsilon_1\right) \simeq \frac{\sigma_2}{\sigma_1}\varepsilon_{21} \tag{50}$$

Thus, at first order, the error $\widetilde{r} - r$ as the following properties:

$$\mathbb{E}\left[\widetilde{r} - r\right] \simeq 0 \tag{51a}$$

$$\operatorname{Var}\left(\widetilde{r} - r\right) \simeq \frac{\sigma_2^2}{\sigma_1^2(N-1)} \tag{51b}$$

We can conclude that:

- As expected, the accuracy of the regression estimation $\widetilde{r}$ increases when the ensemble size N increases.
- For a finite ensemble size N, the relative error of the regression estimation:

$$\frac{\sqrt{\operatorname{Var}\left(\widetilde{r} - r\right)}}{r} \simeq \frac{\sigma_2}{r\sigma_1(N-1)} \tag{52}$$

  can be arbitrary large if on the ratio $\sigma_2/(r\sigma_1)$ is significantly larger than $N-1$. However in this case, equation (40) shows that the correlation coefficient c is close to zero, which means that even a large relative error on $\widetilde{r}$ should not have a strong impact.

Algorithm 1 Recursive computation of the balance operator components using the partial recursive inverse formula

Copy the ensemble perturbations:
for $1 \leq p \leq N$ **do**
  $\delta\widetilde{\mathbf{v}}^p = \delta\widetilde{\mathbf{x}}^p$
end for
for $1 < i \leq m$ **do**
  for $1 \leq j < i$ **do**
    Estimate the covariance between $\mathbf{x}_i$ and $\mathbf{v}_j$:
    $$\widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{v}_j\right) = \frac{1}{N-1}\sum_{p=1}^{N} \delta\widetilde{\mathbf{x}}_i^p \left(\delta\widetilde{\mathbf{v}}_j^p\right)^{\mathrm{T}}$$
    Filter the covariance between $\mathbf{x}_i$ and $\mathbf{v}_j$:
    $$\widehat{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{v}_j\right) = \mathcal{F}\left[\widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{v}_j\right)\right]$$
  end for
  Concatenate matrices to build $\widehat{\mathrm{Cov}}\left(\mathbf{x}_i, \bar{\mathbf{v}}_i\right)$ and $\widehat{\mathrm{Cov}}\left(\bar{\mathbf{v}}_i, \bar{\mathbf{v}}_i\right)$
  Inverse $\widehat{\mathrm{Cov}}\left(\bar{\mathbf{v}}_i, \bar{\mathbf{v}}_i\right)$ to get $\widehat{\mathrm{Cov}}\left(\bar{\mathbf{v}}_i, \bar{\mathbf{v}}_i\right)^{-1}$
  Compute $\overline{\mathbf{K}}_i$:
    $$\overline{\mathbf{K}}_i = \widehat{\mathrm{Cov}}\left(\mathbf{x}_i, \bar{\mathbf{v}}_i\right) \widehat{\mathrm{Cov}}\left(\bar{\mathbf{v}}_i, \bar{\mathbf{v}}_i\right)^{-1}$$
  Update the unbalanced ensemble perturbations:
  for $1 \leq p \leq N$ **do**
    for $1 \leq j < i$ **do**
      $\delta\widetilde{\mathbf{v}}_i^p \leftarrow \delta\widetilde{\mathbf{v}}_i^p - \mathbf{K}_{i,j}\delta\widetilde{\mathbf{v}}_j^p$
    end for
  end for
  if $i < m$ **then**
    for $1 \leq j < i$ **do**
      Estimate the covariance of $\mathbf{v}_i$ with $\mathbf{v}_j$:
      $$\widetilde{\mathrm{Cov}}\left(\mathbf{v}_i, \mathbf{v}_j\right) = \frac{1}{N-1}\sum_{p=1}^{N} \delta\widetilde{\mathbf{v}}_i^p \left(\delta\widetilde{\mathbf{v}}_j^p\right)^{\mathrm{T}}$$
      Filter the covariance of $\mathbf{v}_i$ with $\mathbf{v}_j$:
      $$\widehat{\mathrm{Cov}}\left(\mathbf{v}_i, \mathbf{v}_j\right) = \mathcal{F}\left[\widetilde{\mathrm{Cov}}\left(\mathbf{v}_i, \mathbf{v}_j\right)\right]$$
    end for
  end if
end for

Algorithm 2 Recursive computation of the balance operator components using the full recursive inverse formula

for $1 \leq i \leq m$ **do**
  for $1 \leq j \leq i$ **do**
    Estimate the covariance between $\mathbf{x}_i$ and $\mathbf{x}_j$:
$$\widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{x}_j\right) = \frac{1}{N-1} \sum_{p=1}^{N} \delta\widetilde{\mathbf{x}}_i^p \left(\delta\widetilde{\mathbf{x}}_j^p\right)^{\mathrm{T}}$$
  end for
end for
for $1 < i \leq m$ **do**
  for $1 \leq j < i$ **do**
    Compute the covariance between $\mathbf{x}_i$ and $\mathbf{v}_j$:
$$\widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{v}_j\right) = \sum_{k=1}^{j-1} \widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{x}_k\right) \mathbf{A}_{j,k}^{\mathrm{T}} + \widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{x}_j\right)$$
    Filter the covariance between $\mathbf{x}_i$ and $\mathbf{v}_j$:
$$\widehat{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{v}_j\right) = \mathcal{F}\left[\widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{v}_j\right)\right]$$
  end for
  Concatenate matrices to build $\widehat{\mathrm{Cov}}\left(\mathbf{x}_i, \bar{\mathbf{v}}_i\right)$ and $\widehat{\mathrm{Cov}}\left(\bar{\mathbf{v}}_i, \bar{\mathbf{v}}_i\right)$
  Inverse $\widehat{\mathrm{Cov}}\left(\bar{\mathbf{v}}_i, \bar{\mathbf{v}}_i\right)$ to get $\widehat{\mathrm{Cov}}\left(\bar{\mathbf{v}}_i, \bar{\mathbf{v}}_i\right)^{-1}$
  Compute $\overline{\mathbf{K}}_i$:
$$\overline{\mathbf{K}}_i = \widehat{\mathrm{Cov}}\left(\mathbf{x}_i, \bar{\mathbf{v}}_i\right) \widehat{\mathrm{Cov}}\left(\bar{\mathbf{v}}_i, \bar{\mathbf{v}}_i\right)^{-1}$$
  for $1 \leq j < i$ **do**
    Compute the matrix $\mathbf{A}_{i,j}$:
$$\mathbf{A}_{i,j} = -\sum_{k=j}^{i-1} \mathbf{K}_{i,k} \mathbf{A}_{k,j}$$
  end for
  if $i < m$ **then**
    for $1 \leq j < i$ **do**
      Compute temporary matrices $\mathbf{S}_{k,j}$:
      for $1 \leq k \leq i$ **do**
$$\mathbf{S}_{k,j} = \sum_{l=1}^{k} \widetilde{\mathrm{Cov}}\left(\mathbf{x}_k, \mathbf{x}_l\right) \mathbf{A}_{j,l}^{\mathrm{T}} + \sum_{l=k+1}^{j-1} \widetilde{\mathrm{Cov}}\left(\mathbf{x}_l, \mathbf{x}_k\right)^{\mathrm{T}} \mathbf{A}_{j,l}^{\mathrm{T}} + \widetilde{\mathrm{Cov}}\left(\mathbf{x}_k, \mathbf{x}_j\right)$$
      end for
      Compute the covariance between $\mathbf{v}_i$ and $\mathbf{v}_j$:
$$\widetilde{\mathrm{Cov}}\left(\mathbf{v}_i, \mathbf{v}_j\right) = \sum_{k=1}^{i-1} \mathbf{A}_{i,k} \mathbf{S}_{k,j} + \mathbf{S}_{i,j}$$
      Filter the covariance between $\mathbf{v}_i$ and $\mathbf{v}_j$:
$$\widehat{\mathrm{Cov}}\left(\mathbf{v}_i, \mathbf{v}_j\right) = \mathcal{F}\left[\widetilde{\mathrm{Cov}}\left(\mathbf{v}_i, \mathbf{v}_j\right)\right]$$
    end for
  end if
end for

Algorithm 3 Recursive computation of the balance operator components using the full recursive inverse formula, with an extra covariance averaging step

for $1 \leq i \leq m$ **do**
  for $1 \leq j \leq i$ **do**
    Estimate the covariance between $\mathbf{x}_i$ and $\mathbf{x}_j$:
$$\widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{x}_j\right) = \frac{1}{N-1}\sum_{p=1}^{N} \delta\widetilde{\mathbf{x}}_i^p \left(\delta\widetilde{\mathbf{x}}_j^p\right)^{\mathrm{T}}$$
    Read old covariance estimate $\widetilde{\mathrm{Cov}}_{\mathrm{old}}\left(\mathbf{x}_i, \mathbf{x}_j\right)$ and average with the current covariance estimate:
$$\widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{x}_j\right) \leftarrow \alpha\widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{x}_j\right) + (1-\alpha)\widetilde{\mathrm{Cov}}_{\mathrm{old}}\left(\mathbf{x}_i, \mathbf{x}_j\right)$$
  end for
end for
As algorithm 2 from this point onwards.